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Time Monday, March 5, 2001

1:00 pm - 2:00 pm

Location 50D-4205 Conference Room**Title** Low-frequency normal modes of proteins**Lecturer** Yves-Henri Sanejouand, [CRPP - Centre de Recherche Paul-Pascal](#), Pessac, France

Abstract A lot of information on the nature of the functional motions of proteins is often found in their lowest-frequency normal modes, as they are obtained following normal mode theory. Until recently, however, the calculation of such modes for large or even average-size proteins was not a straightforward task.

Two approaches allowing for such calculations on common workstations will be described in this talk. In the first one, called RTB (standing for Rotation-Translation-of-Blocks), low-frequency normal modes of proteins are assumed to be well described as pure rigid-body motions of consecutive amino-acids (1). In the second one, they are calculated using a very simplified one-parameter protein model (2). It will be shown that both methods yield results in very good agreement with standard ones, allowing to obtain accurate insights on the kind of functional motion a protein can perform.

References: 1) Tama, Gadea, Marques, Sanejouand (2000): "Building-block approach for determining low-frequency normal modes of macromolecules", *Proteins*, vol.41, p1-7. 2) Tama, Sanejouand (2001): "Conformational change of proteins arising from normal mode calculations", to appear in *Protein Engineering*.

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